Linking Probabilities of Self-Avoiding Polygons

Naomi Hirayama† * , Kyoichi Tsurusaki‡, Tetsuo Deguchi† †Graduate School of Humanities and Sciences, Ochanomizu University, ‡Kanagawa Industrical Technology Center, †2-1-1 Ohtsuka, Bunkyo-ku, Tokyo, 112-8610, Japan, ‡705-1 Shimoimaizumi, Ebina-shi, Kanagawa, 243-0435, Japan, †Tel: +81-3-5978-5313

We have numerically investigated the probability $P_L(r)$ for a pair of self-avoiding random polygons (SAPs) being link L such that each of them have the trivial knot type and they have no overlaps among the segments where they are placed with a distance r between the centers of mass. We call it the linking probability of link L. We propose the following fitting formula: $P_L(r) = \exp(-\alpha r^{\nu}) - C\exp(-\beta r^{\mu})$, where α, ν, C, β and μ are parameters. For example, $P_{0_1^2}(r)$ denotes the probability of the trivial link. We apply the formula also to the data of $P_{link}(r)$, where it is given by $P_{link}(r) = 1 - P_{0_1^2}(r)$. With respect to the χ^2 values, the formula gives good fitting curves to the values of $P_{link/L}(r)$ versus r obtained by simulation for $r_d \leq 0.20$. In the simulation we generate SAPs consisting of N spherical segments of radius r_d, where the bond length, i.e the distance between adjacent segments, is fixed to 1. We have numerically obtained $P_{link/L}(r)$ for the cases of $N = 32$, 64, 128 and 256 for $r_d = 0.00, 0.05, \cdots, 0.30$.

本研究では，環状高分子の溶液やネットワークの性質に深く関係する絡み合い確率を数値的に評価して考察した。絡み合い確率 $P_L(r)$ は，2つの環状高分子を重心間距離 r だけ離して置いた場合に，それらがリンク・タイプ L のトポロジーを持って絡み合う確率である。また，環状鎖が非自明な絡み目をつくる確率を $P_{link}(r)$ と表す。我々は，環状鎖の長さや排除体積を変えてシミュレーションを行い，$P_L(r)$ および $P_{link}(r)$ の評価を行った。その結果，これらは距離の関数としては次の関数型: $P_{link/L} = \exp(-\alpha r^{\nu}) - C\exp(-\beta r^{\mu})$ で表されることが分かった。ここで α, ν, C, β, μ は適合変数である。上記の関数は L によらず一般的に成り立つ。さらに，排除体積が極限的に大きい場合を除いて，上式が計算結果を良く再現することが χ^2 値のからも裏付けられた。

1 Introduction

Recently, a number of experimental techniques have been developed and ring polymers and catenanes have been synthesized by various researchers (see [1], for instance). In the systems of ring polymers conservation of the topology plays an important role in the statistical and dynamical properties. The linking probability should be fundamental to understand the entropic behavior of topologically restricted polymers such as ring polymers.

Suppose that we have a pair of SAPs that have no overlaps among the segments when the centers of mass are separated by a distance r, and also that each of the SAPs has the trivial knot type. We define the linking probability $P_L(r)$ by the probability that such a pair of SAPs has link type L. Here, r is normalized by the root-mean-square radius of gyration of the SAP. We denote by $P_{0_1^2}$ the probability of the trivial link. We also define the linking probability $P_{link}(r)$ by the probability that two such SAPs make a non-trivial link. In other words, we have $P_{link} = \sum_{L\neq 0_1^2} P_L = 1 - P_{0_1^2}$.

*E-mail: nezuri@degway.phys.ocha.ac.jp

Although various formulas of $P_{link/L}$ as functions of r have been suggested (see [2] and [3], for instance), they do not give good fitting curves to the simulation results of $P_{link/L}(r)$ with sufficiently small χ^2 values. In this paper, we propose a new formula:

$$P_{link/L}(r) = \exp(-\alpha r^{\nu}) - C\exp(-\beta r^{\mu}), \qquad \alpha,\ \nu,\ C,\ \beta \text{ and } \mu\text{: fitting parameters.} \tag{1}$$

We also show numerically how linking probability $P_{link/L}(r)$ depends on the excluded-volume.

In Section 2, we explain numerical methods of the present work in detail. The validity of the formula is confirmed in Section 3. Finally, the main results and conclusions are summarized in Section 4.

2 Procedure of simulations

We generate SAPs using the crank-shaft algorithm. It is similar to the pivot algorithm on a lattice [4]. The procedure is given as follows. Let us begin with a regular polygon of N nodes. In the polygon, the beads of radius r_d are located at all nodes and the bond length is given by 1. Under the self-avoiding conditions, the beads are not allowed to overlap with each other. First, we randomly choose two nodes of the polygon. Next, we rotate a sub-chain between the two nodes around the axis through them. Here the rotation angle is given by a random number. We then check all nodes whether they overlap or not. If the nodes have no overlaps, the conformation is accepted as a new one. On the other hand, if a pair of the nodes has an overlap, we return the polygon to the state before the deformation. We repeat the procedure many times. Finally, we employ the polygon as a member of an ensemble of SAP when it has an effectively independent conformation from the initial one. We should comment that an independent conformation can be practically obtained if successful deformation is repeated about N times. In the present work, we perform such deformation $2N$ times to generate a SAP.

We define a self-avoiding random link by such a pair of two SAPs that have no overlaps and are put at a normalized distance r between the centers of mass. Here, we assume that the two SAPs have the same N and r_d and both of them have the trivial knot type. They are randomly chosen from an ensemble of such SAPs. We produce 10^5 self-avoiding random links to estimate $P_L(r)$.

The linking probability $P_L(r)$ with link type L is calculated by

$$P_L(r) = \frac{M_L}{M} \tag{2}$$

where M_L is the number of self-avoiding random links with link type L and M is the total number of all self-avoiding links, which is given by 10^5 in our simulation.

To detect the link types of the 10^5 self-avoiding random links, we use two link invariants: the linking number and the Alexander polynomial. By the invariants, we have practically classified the link types such as 0_1^2, 2_1^2, 4_1^2 and 5_1^2 (Fig 1).

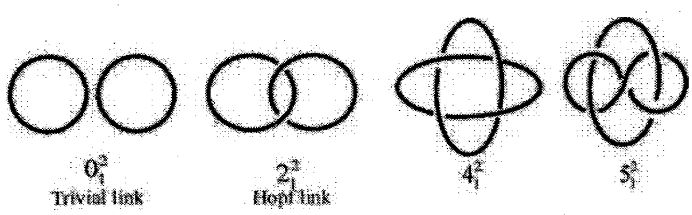
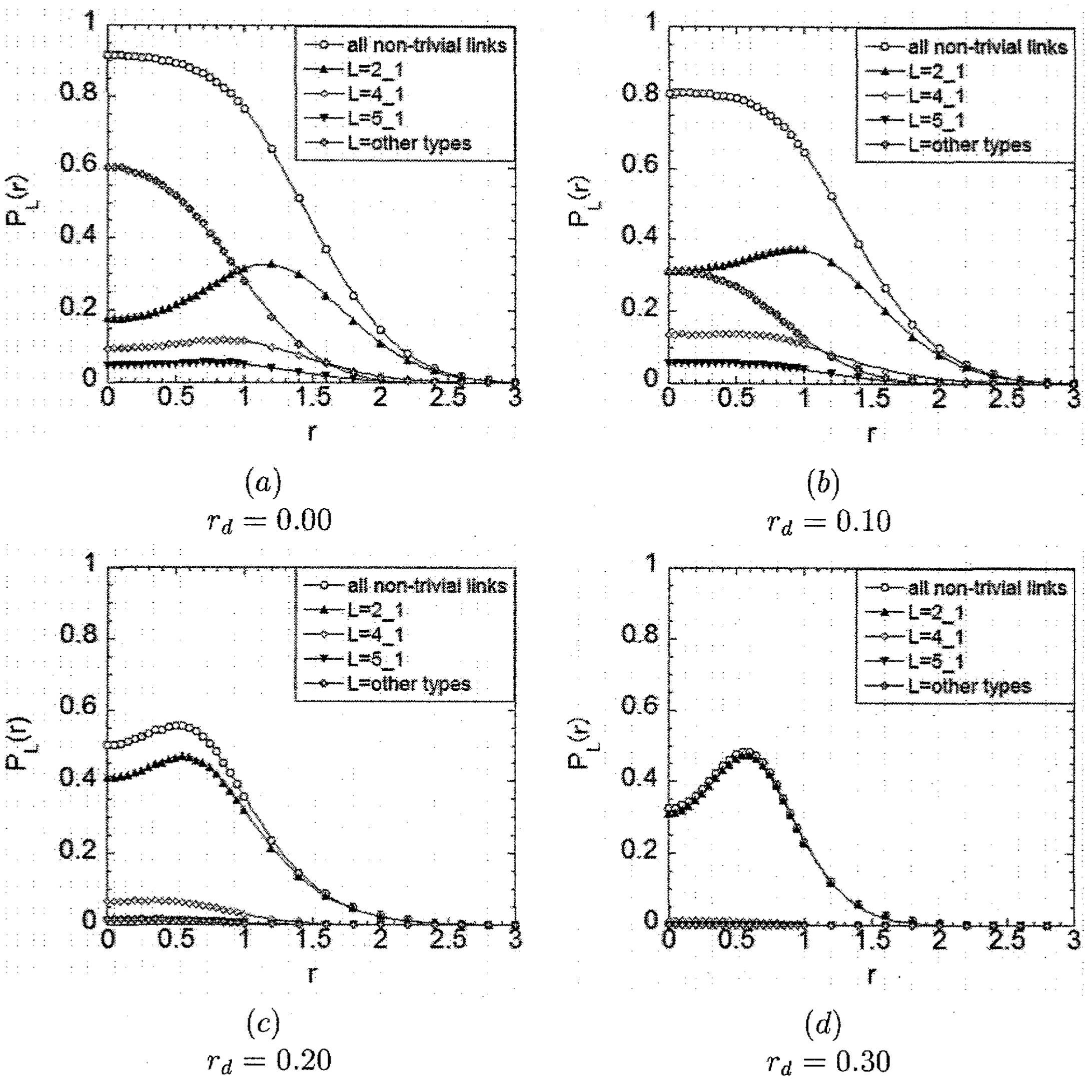


Figure 1: Some link types

3 Results

The simulation results of $P_{link/L}(r)$ as a function of r are plotted in Fig. 2 for the case of $N = 256$ for $r_d = 0.0$, 0.1, 0.2 and 0.3. The solid lines are fitting curves given by formula (1). Fig. 2 shows that formula (1) is consistent with the data.



(a) $r_d = 0.00$ (b) $r_d = 0.10$

(c) $r_d = 0.20$ (d) $r_d = 0.30$

Figure 2: **Linking probabilities $\mathbf{P_{link/L}(r)}$ with $\mathbf{N = 256}$** Data points of "all non-trivial links" denote those of linking probability $P_{link}(r)$. $P_{2_1^2}(r)$, $P_{4_1^2}(r)$ and $P_{5_1^2}(r)$ are the probabilities of link types 2_1^2, 4_1^2 and 5_1^2. And $P_{other\,types}(r)$ denotes the probability that a given self-avoiding random link is equivalent to a non-trivial link other than 2_1^2, 4_1^2 and 5_1^2.

The χ^2 values are listed in Table 1. Note that there are 31 points on each curve. The χ^2 values are sufficiently small for all the cases of $r_d \leq 0.20$. Furthermore, simulation results for the cases of $N = 32$, 64 and 128 are also approximated by the formula (1) with small χ^2 values. From the results, we conclude that formula (1) gives good fitting curves to the estimates of $P_{link/L}(r)$ as a function of r with respect to the χ^2 values for $r_d \leq 0.20$.

L	$rd = 0.00$	$rd = 0.05$	$rd = 0.10$	$rd = 0.15$	$rd = 0.20$	$rd = 0.25$	$rd = 0.30$
$link$	43.4	33.3	13.0	12.2	51.3	143.	267.
2_1^2	16.7	17.4	10.1	13.4	37.1	153.	233.
4_1^2	8.00	9.20	33.5	42.6	21.8	15.5	7.80
5_1^2	12.2	9.20	13.8	8.60	5.60	-	-

Table 1: χ^2 **values of** $\mathbf{P_{link/L}(r)}$ **for** $\mathbf{N = 256}$ From the fitting curves of $P_{link/L}(r)$ given by formula (1), we obtain the χ^2 values for the case of $N = 256$ for $r_d = 0.00, 0.05, \cdots$, and 0.30. It was not possible to evaluate the χ^2 values for the case of $L = 5_1^2$ for $r_d = 0.25$ and 0.30 because the numerical values of $P_{5_1^2}(r)$ are almost 0.

We have investigated the excluded-volume dependence of $P_{link/L}(r)$. In Fig. 2, we found that $P_L(r)$ of $L = 4_1^2, 5_1^2$ and *other types* decrease quickly for all values of r when r_d increases for $r_d \geq 0.20$. However, only $P_{2_1^2}(r)$ does not vanish when r_d is large such as $r_d = 0.30$. That is, almost all the self-avoiding random links of non-trivial link types have the link type 2_1^2 for $r_d \geq 0.30$.

Furthermore, we found that the graph of $P_{2_1^2}(r)$ has a peak for all values of r_d, and also that the peak position approaches $r \approx 0.5$ as r_d increases for $r_d \geq 0.20$.

4 Conclusions

We proposed formula (1) to express linking probabilities P_{link} and P_L as a functions of r for some link types such as $L = 2_1^2$, 4_1^2 and 5_1^2. With respect to the χ^2 values, formula (1) is consistent with the simulation data at least in the case of $r_d \leq 0.20$.

We found that when the excluded-volume is very large, probabilities P_L of non-trivial links L vanish except for $P_{2_1^2}$. Moreover, the value of $P_{2_1^2}$ remains constant when r_d increases for $r_d \geq 0.20$.

References

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